IN THE CLAIMS:

Please cancel claim 16 without prejudice. This listing of claims replaces all prior versions and listings of claims in the application:

Listing of Claims

1-8 (Canceled)

9. (Withdrawn) A computer-assisted method for determining a three-dimensional structure of a target protein using a computer comprising a processor configured to receive and output data in accordance with executable code, the method comprising:

(a) generating input data for the computer comprising:

(i) inputting as a string of an identity constraint and a secondary structure constraint and/or tertiary constraints for some or all of the amino acid residues residue comprising the target protein; and

(ii) by way of executable code, directing the processor to produce from the string a three dimensional reduced protein model comprised of representations of side chains of the amino acid residues comprising the target protein; and

(b) outputting the three dimensional reduced protein model to an output device or a storage device.

10. (Withdrawn) A method according to claim 9 wherein the secondary structure constraint for each amino acid residue is selected from the group of "H" for helix, "E" for extended, and "(-)" for other structural constraints.

11. (Withdrawn) A method according to claim 9 wherein the secondary structural constraint for a subset of amino acid residues comprising the target protein is generated by a threading alignment of an amino acid sequence of the target protein.

12. (Withdrawn) A computer-assisted method for determining a three-dimensional structure of a target amino acid sequence, the method comprising inputting into the computer an alignment of a target amino acid sequence with a template amino acid sequence and calculating with the said computer one or more three-d8imensional reduced protein model comprising representations of side chains of amino acid residues comprising a target protein.

13. (Withdrawn) A method according to claim 12 further comprising outputting to an output device or a storage device one or more of the three-dimensional reduced protein models.

14. (Previously Presented) A computer-assisted method for determining a three-dimensional structure of a target amino acid sequence using a computer comprising a processor configured to receive and output data in accordance with executable code, the method comprising:

(a) generating input data for the computer comprising:

(i) inputting into the computer an alignment of a target amino acid sequence with a template amino acid sequence; ~~and~~

(ii) by way of executable code, directing the processor to

produce from the ~~alignment a three-dimensional reduced protein model~~ template amino acid sequence ~~comprising~~ a template representations of side chains of amino acid residues ~~comprising a target protein, wherein said representations of side chains of amino acid residues are~~ converted to a plurality of interaction centers, ~~and~~ wherein each interaction center comprises a pseudoatom representing a center of mass of the side chain of the represented amino acid to which the interaction center corresponds, and each interaction center is

connected to an immediately proximal interaction center and an immediately distal interaction center via a virtual covalent bond to produce ~~an~~ a template interaction center chain, which is projected onto an underlying cubic lattice to produce a projected chain of interaction centers, and then secondary constraints and/or tertiary constraints are applied to a subset of, or all of, the interaction centers of the interaction center chain to generate a force field comprising short-range interactions, thereby producing a data set representing a three-dimensional model structure of the target protein; and

(iii) produce from the target amino acid sequence, beginning at the first aligned position with the template amino acid sequence, a target representations of side chains of amino acid residues converted to a plurality of interaction centers, wherein each interaction center comprises a pseudoatom representing a center of mass of the side chain of the represented amino acid to which the interaction center corresponds, and each interaction center is connected to an immediately proximal interaction center and an immediately distal interaction center via a virtual covalent bond to produce an target interaction center chain, which is projected onto an underlying cubic lattice to produce a projected chain of interaction centers, and then secondary constraints and/or tertiary constraints are applied to a subset of, or all of, the interaction centers of the interaction center chain to generate a force field comprising short-range interactions, thereby producing a data set representing a three-dimensional model structure of the target protein, and minimizing the distance of the target interaction center chain from the equivalent template points, wherein a gap in the alignment of the template and target amino acid sequences is divided to generate a set of check points, wherein the checkpoints equal the number of target amino acid residues that span the gap region; and

(b) outputting the three-dimensional reduced protein model to an output device or a storage area.

15. (Previously Presented) The method of claim 14, wherein producing the data set representing a three-dimensional model structure of the target protein comprises determining side chain center of mass positions of amino acid residues of the target protein by generating a

force field comprising short-range interactions that reflect secondary structure propensities and short-range packing biases.

16. (Canceled)

17. (Currently Amended) The method of claim 14 ~~or claim 16~~, wherein the executable code comprises instructions for:

connecting said interaction centers by virtual covalent bonds, wherein each interaction center comprises a pseudoatom representing a center of mass of the side chain of the represented amino acid to which the interaction center corresponds, and wherein each interaction center, except for the interaction centers representing the amino and carboxy terminal amino acid residues of the target protein, is connected to an immediately proximal interaction center and an immediately distal interaction center via a virtual covalent bond to produce an interaction center chain.

18. (Previously Presented) The method of claim 17 wherein the executable code further comprises projecting the interaction center chain onto an underlying cubic lattice to produce a projected chain on interaction centers.

19. (Previously Presented) The method of claim 18 wherein the executable code further comprises applying secondary constraints and/or tertiary constraints to a subset of interaction centers of the interaction center chain so as to produce a data set representing a three-dimensional model structure of the target protein.

20. (Currently Amended) The method of claim 14 ~~or claim 16~~, wherein the executable code comprises instructions for:

(a) connecting said interaction centers by virtual covalent bonds, and wherein each interaction center, except for the interaction centers representing the amino and carboxy

terminal amino acid residues of the target protein, is connected to an immediately proximal interaction center and an immediately distal interaction center via a virtual covalent bond to produce an interaction center chain; and

(b) projecting the interaction center chain onto an underlying cubic lattice to produce a projected chain on interaction centers;

(c) applying secondary constraints or tertiary constraints, or, secondary constraints and tertiary constraints, to a subset of interaction centers of the interaction center chain so as to produce a data set representing a three-dimensional model structure of the target protein.

21. (Currently Amended) The method of claim 14 ~~or claim 16~~, wherein the target amino acid sequence comprises a sequence of less than all of the amino acid residues of a protein.

22. (Currently Amended) The method of claim 14 ~~or claim 16~~, wherein the target amino acid sequence comprises a sequence of all of the amino acid residues of a protein.

23. (Currently Amended) The method of claim 14 ~~or claim 16~~, wherein the interaction center comprises a pseudoatom representing a center of mass of a side chain.

24. (Previously Presented) The method of claim 15, further comprising combining the force field with a small number of long-range harmonic constraints to generate a three-dimensional model structure of the target protein.

25. (Currently Amended) The method of claim 14 ~~or claim 16~~, wherein the method is iteratively repeated to generate a three-dimensional model structure of the target protein.